Final Technical Report for Grant N00014-89-J-2018
Linear and Nonlinear Optical Properties of Quantum Dots

K. M. Leung

Polytechnic University
Department of Physics, Brooklyn, NY, 11201

ABSTRACT

1990

is calculated for

We calculated the dispersion relation ~~of~~ artificial optical media consisting of periodic arrays of microparticles embedded in a host medium. Our major objective is to utilize photonic bandgap engineering techniques to modifify the optical modes in such a way that will drastically alter many optical and electronic processes.

1. Motivations

Electromagnetism is the fundamental force in Nature that governs much of the low energy phenomena of atomic, molecular and condensed-matter systems. These phenomena can therefore be substantially altered by utilizing three-dimensional periodically modulated dielectric structures to controllably modify the relevent optical modes. Particular interest is on structures containing periodic arrays of nondissipative high dielectric constant microparticles of size and inter-particle spacing comparable to the wavelength of the optical modes of interest. The goal is to create an artificial optical medium that scatters light so strongly that a bandgap exist over a finite frequency range irrespective of the propagation direction.[1] [2] [3] There are many important applications of such novel meterials. (1) Since electromagnetic modes are totally absent within the bandgap, spontaneous emission is therefore strongly suppressed. This ability to inhibit spontaneous emission has some extremely important consequences since spontaneous emission plays a fundamental role in

limiting the performance of many optical and electronic devices such as semiconductor lasers, heterojunction bipolar transistors, and solar cells. [1] [4] The inhibition of spontaneous emission of a Rydberg atom in a microwave cavity has in fact been demonostrated. [5] [6] [7] Unfortunately, the basic setup is extremely difficult to implement for practical applications. In contrast, our approach here is from a purely material engineering point of view, and should be easily applicable. (2) The fundamental properties of many atomic and molecular, and excitonic systems can be profoundly modified in a volume of space where the most important electromagnetic processes are totally absent. [8] (3) There is also a proposal to study mobility edges and Anderson localization of photons within a pseudo-gap which can be obtained with the introduction of randomness. [2]

2. *Scalar Wave Calculation*

We have published results using both the Korringa-Kohn-Rostoker (KKR) and plane wave method for the band structure of a face-centered cubic array of spherical microparticles for various dielectric contrast, r and volume filling fraction of microparticles, f. [9] Our numerical results based on the two entirely different methods agree extremely well. We show that a commom photonic gap can in fact exist in such materials, and it persists down to an r value of about 2.9. We also find that the optimal value of f depends significantly on the value of r, and in general decreases with increasing r. In addition, our plane wave calculation is found to converge fairly rapidly. This is an important finding since the plane wave method is comparatively much simplier than the KKR method, the computer program is much easier to write, and runs substantially much faster. Moreover, unlike the KKR method, which is limited to "muffin-tin"-like modulation of the "potential", the plane wave method can readily handle all sorts of modulations. This capability is especially important since we believe that, besides requiring a high dielectric contrast, the shape of the dielectric structure is also a very crucial factor in determining the photon band structure and the existence of a gap in the density of states.

3. Full Vector Calculation

To our knowledge, our work [10] is the first to report the photonic band structures in three dimensionally periodic dielectric media based on exact full vector wave calculations. Our numerical method employs plane wave expansions. The structure we studied is the same as that investigated experimentally, [3] and in our previous scalar wave calculation. The band structure is computed for various values of r and f. In particular, we have also studied the case in which the spheres are air-atoms which are so closely packed that they are actually overlapping. This case is especially interesting in that it was found experimentally to have a common photon band gap throughout the entire Brillouin zone. Overall our theoretical results are in reasonable agreement with those of the experiment.[3] This includes the effective long wavelength refractive index as a function of the volume filling fraction, and the size of the gap at the L- and X-points within the first Brillouin zone for the sample with an 86% of air-atoms. However, there is a discrepancy for this case at the W-point, where our result suggests that a gap does not exist because of symmetry. In addition, in the W to K direction away from the W-point, the gap is much more feeble than measured experimentally.

After extensive numerical calculations for r ranging from 1/4 to 4, and for various volume filling fractions we did not find a common gap for spherical microparticles in this face-centered cubic geometry. In order to create a common photonic gap, our work suggests that it is important to introduce a mechanism which will either redistribute the strength of the Fourier coefficients of the potential in such a way that degenerate levels at the W point do not occur for the second and third levels, or perturb the shape of the microparticles and/or deviate from the face-centered cubic symmetry so as to lift the degeneracy of these levels.

REFERENCES

1. E. Yablonovitch, Phys. Rev. Lett. **20**, 2059 (1987).

2. S. John and R. Rangarajan, Phys. Rev. B **38**, 10101 (1988).

3. E. Yablonovitch and T. J. Gmitter, Phys. Rev. Lett. **18**, 1950 (1989).

4. E. Yablonovitch, T. J. Gmitter, and R. Blat, Phys. Rev. Lett. **22**, 2546 (1988).

5. R. G. Hulet, E. S. Hifer, and D. Kleppner, Phys. Rev. Lett. **55**, 2137 (1985).

6. W. Jhe, A. Anderson, E. A. Hinds, D. Meschede, L. Moi, and S. Haroche, Phys. Rev. Lett. **58**, 1320 (1987).

7. D. J. Heinzen and M. S. Feld, Phys. Rev. Lett. **59**, 2623 (1987).

8. G. Kurizki and A. Z. Genack, Phys. Rev. Lett. **61**, 2269 (1988).

9. K. M. Leung and Y. F. Liu, Phys. Rev. **B41**, 10188 (1990).

10. K. M. Leung and Y. F. Liu, to be published.